Ensemble Learning

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Introduction to Ensemble Learning

Ensemble Methods

Use multiple models for prediction.
Most winning entries of Kaggle competitions use ensemble learning.

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Example:
Classifier 1 - Good
Classifier 2 - Good
Classifier 3 - Bad

Using Majority Voting, we predict Good.

Ensemble Methods

Use multiple models for prediction.
Most winning entries of Kaggle competitions use ensemble learning.

Example:
Regressor 1 - 20
Regressor 2 - 30
Regressor 3 - 30

Using averaging, we predict $\frac{80}{3}$

Intuition

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Based on Ensemble methods in ML by Dietterich
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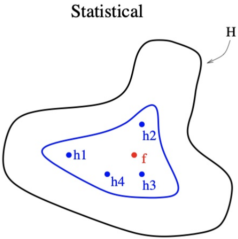
Three reasons why ensembles make sense:
1) Statistical: Sometimes if **data is limited, many competing hypotheses can be learned** all giving the same accuracy on training data.
E.g., we can learn many decision trees for the same data giving the same accuracy.



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2) Computational: Even if data is sufficient, some **classifiers/regressors can get stuck in local optima or apply greedy strategies**. Computationally learning the “best” hypothesis can be non-trivial.

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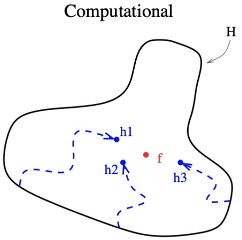
E.g., decision trees employ greedy criteria



Intuition

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3) Representational: Some **classifiers/regressors cannot learn the true form or representation.**

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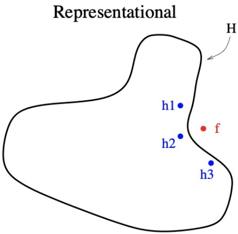
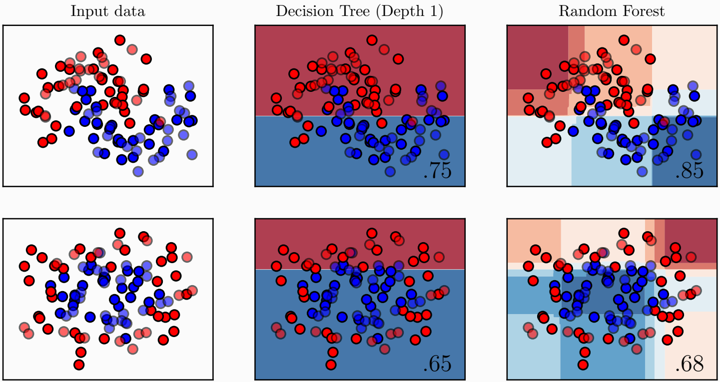
E.g., decision trees can only learn axis-parallel splits.



Representation of Limited Depth DTs vs RFs

Notebook: ensemble-representation.html



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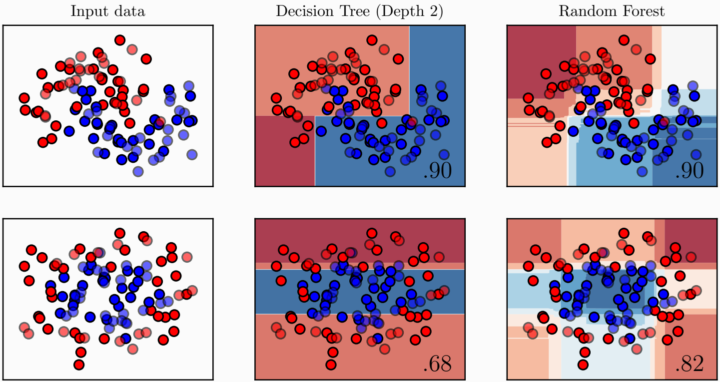

Necessary and Sufficient Conditions

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2) An accurate classifier: is one that has an error rate of better than random guessing on new x values.
3) Two classifiers are diverse: if they make different errors on new data points

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Necessary and Sufficient Conditions

Imagine that we have an ensemble of three classifiers (h_1, h_2, h_3) and consider a new case x.
If the three classifiers are identical, i.e. not diverse, then when $h_1(x)$ is wrong $h_2(x)$ and $h_3(x)$ will also be wrong.
However, if the errors made by the classifiers are uncorrelated, then when $h_1(x)$ is wrong, $h_2(x)$ and $h_3(x)$ may be correct, so that a majority vote will correctly classify.

Intuition for Ensemble Methods from Quantitative Perspective

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Error Probability of each model $= \varepsilon = 0.3$

$Pr(\text{ensemble being wrong}) =$
${}^3C_2(\varepsilon^2)(1-\varepsilon)^{3-2} + {}^3C_3(\varepsilon^3)(1-\varepsilon)^{3-3}$

$$= 0.19 \leq 0.3$$

Some calculations

Number of Models	Ensemble Error	Individual Error
1	0.3	0.3
3	0.216	0.3
5	0.163	0.3

Some calculations

Number of Models	Ensemble Error	Individual Error
1	0.6	0.6
3	0.648	0.6
5	0.683	0.6

Ensemble Methods

Where does ensemble learning not work well?

Ensemble Methods

Where does ensemble learning not work well?

- The base model is bad.
- All models give similar prediction or the models are highly correlated.

Bagging

Also known as *Bootstrap Aggregation*.

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Key idea : Reduce Variance

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Think about cross-validation!

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Think about cross-validation!

We will create multiple datasets from our single dataset using "*sampling with replacement*".

Bagging

Consider our dataset has n samples: $D_1, D_2, D_3, \ldots, D_n$.
For each model in the ensemble, we create a new dataset of size n by sampling uniformly with replacement.

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Round 1: $D_1, D_3, D_6, D_1, \ldots, D_n$
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Repetition of samples is possible.

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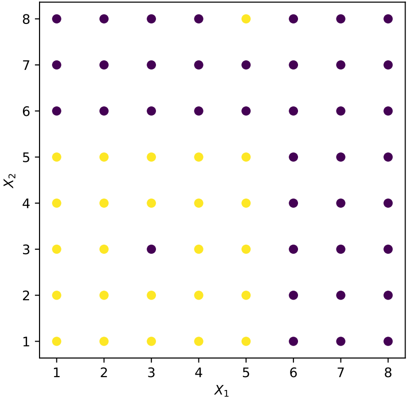
Repetition of samples is possible.
We can train the same classifier/models on each of these different "Bagging Rounds".

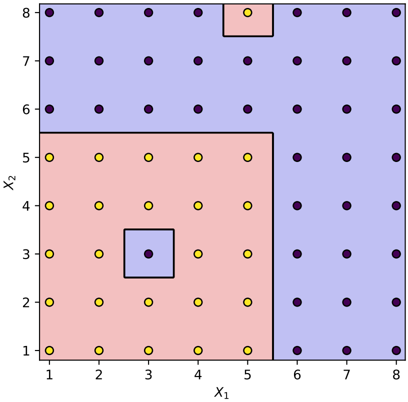
Bagging : Classification Example

Consider the dataset below. Points (3,3) and (5,8) are anomalies.



Bagging : Classification Example

Decision Boundary for decision tree with depth 6.



Bagging : Classification Example

Let's use bagging with an ensemble of 5 trees.

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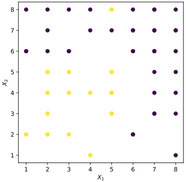

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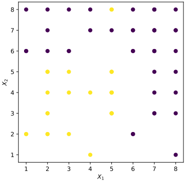
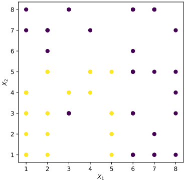


Round - 2



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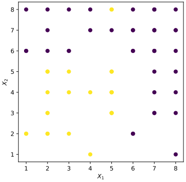

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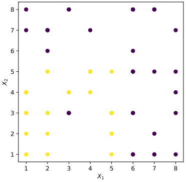
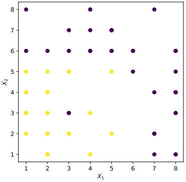


Round - 3



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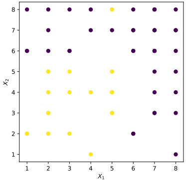

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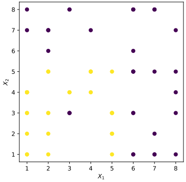

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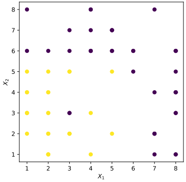
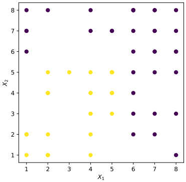


Round - 4



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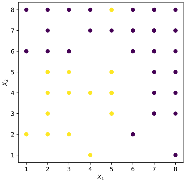

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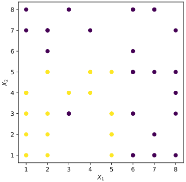

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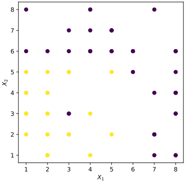
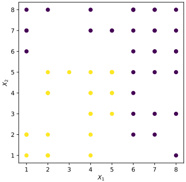
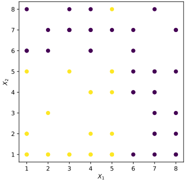


Round - 4



Round - 5



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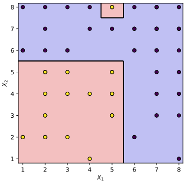
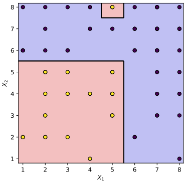


Tree Depth = 4

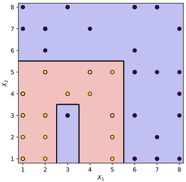
Bagging : Classification Example

Round - 1



Tree Depth = 4

Round - 2



Tree Depth = 5

Bagging : Classification Example

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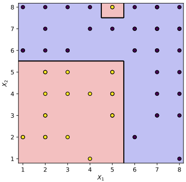

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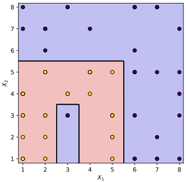
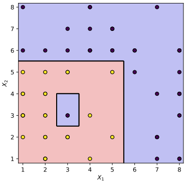
Round - 2



Tree Depth = 5

Round - 3



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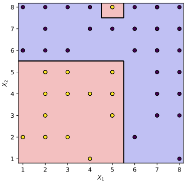
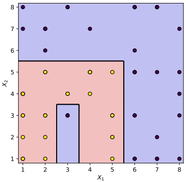


Tree Depth $= 4$

Round - 2



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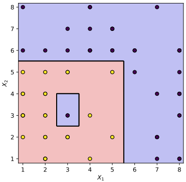
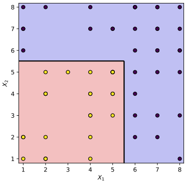


Tree Depth $= 5$

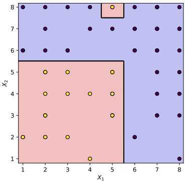
Round - 4



Tree Depth $= 2$

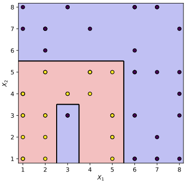
Bagging : Classification Example

Round - 1



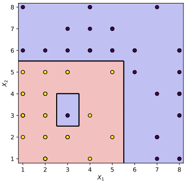
Tree Depth = 4

Round - 2



Tree Depth = 5

Round - 3



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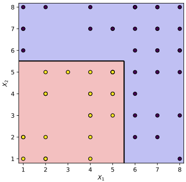
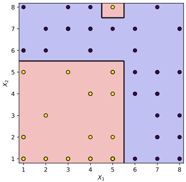
Round - 4



Tree Depth = 2

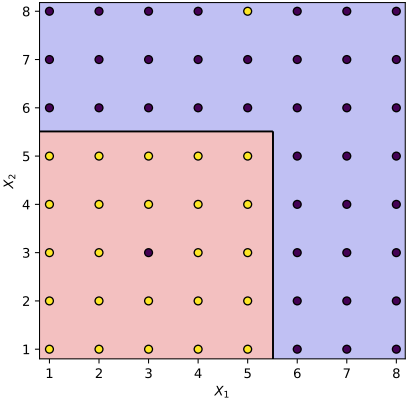
Round - 5



Tree Depth = 4

Bagging : Classification Example

Using majority voting to combine all predictions, we get the decision boundary below.



Bagging

Summary

- We take “strong” learners and combine them to reduce variance.
- All learners are independent of each other.

Boosting

- We take "weak" learners and combine them to reduce bias.

Boosting

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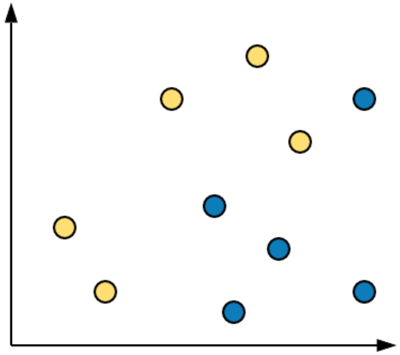
- All learners are incrementally built.

Boosting

- We take "weak" learners and combine them to reduce bias.
- All learners are incrementally built.
- Incremental building: Incrementally try to classify "harder" samples correctly.

Boosting : AdaBoost

Consider we have a dataset of N samples.
Sample i has weight w_i. There are M classifiers in the ensemble.



Boosting : AdaBoost

Consider we have a dataset of N samples.
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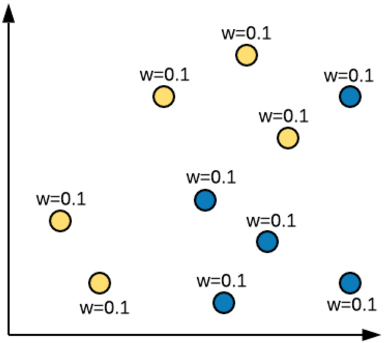
1. Initialize weights of data samples: $w_i = \frac{1}{N}$



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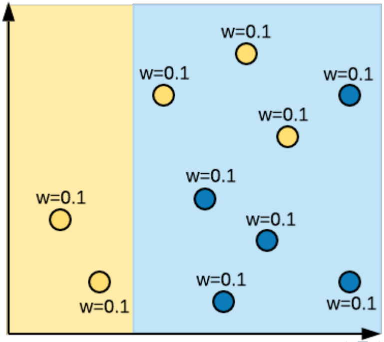
   1) Learn classifier using current weights w_i's



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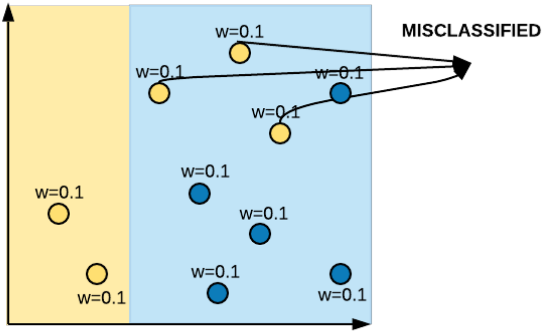

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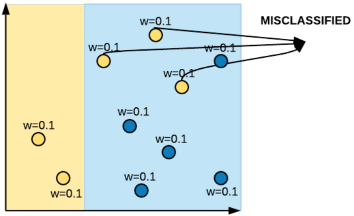
2. For $m = 1, \ldots, M$:
   1) Learn classifier using current weights w_i's
   2) Compute the weighted error: $\text{err}_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$



$$err_1 = \frac{0.3}{1}$$

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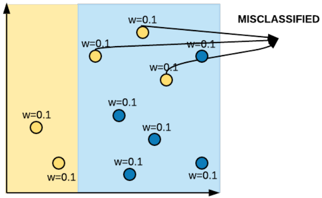
   3) Compute $\alpha_m = \frac{1}{2} \log_e \left(\frac{1-\text{err}_m}{\text{err}_m} \right)$



$$err_1 = \frac{0.3}{1}$$
$$\alpha_1 = \frac{1}{2} log \left(\frac{1-0.3}{0.3} \right) = 0.42$$

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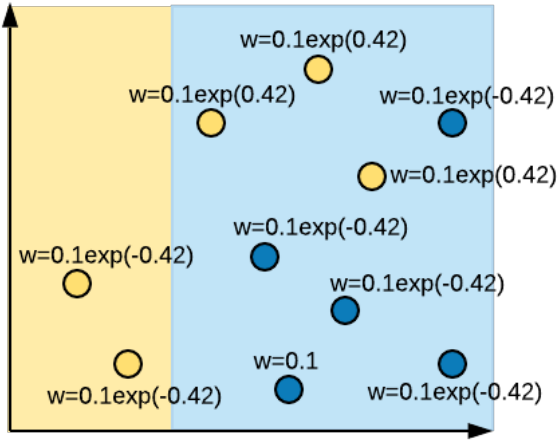
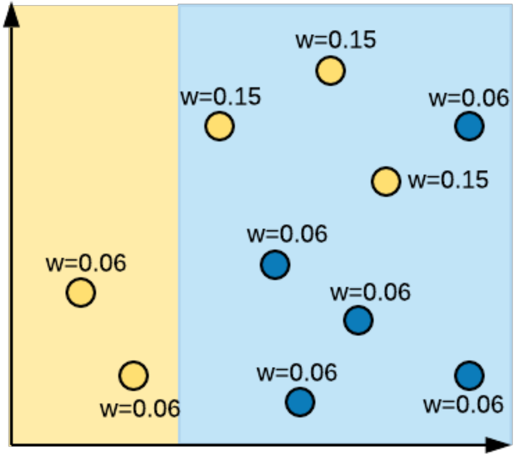
    1) Learn classifier using current weights w_i's
    2) Compute the weighted error: $\text{err}_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$
    3) Compute $\alpha_m = \frac{1}{2} \log_e \left(\frac{1 - \text{err}_m}{\text{err}_m} \right)$
    4) For samples which were predicted correctly: $w_i = w_i e^{-\alpha_m}$
    5) For samples which were predicted incorrectly: $w_i = w_i e^{\alpha_m}$

Boosting : AdaBoost



Boosting : AdaBoost

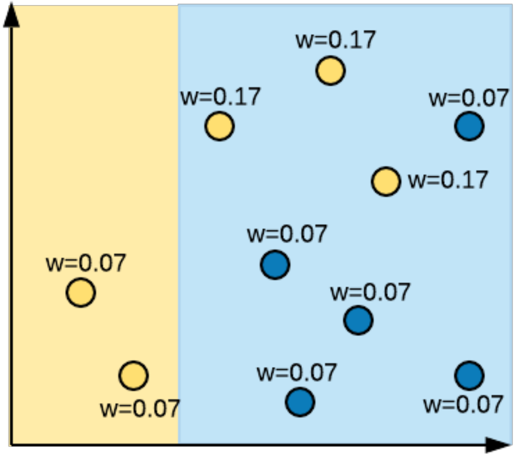


Boosting : AdaBoost

Consider we have a dataset of N samples.
Sample i has weight w_i. There are M classifiers in the ensemble.

1. Initialize weights of data samples: $w_i = \frac{1}{N}$
2. For $m = 1, \ldots, M$:
   1) Learn classifier using current weights w_i's
   2) Compute the weighted error: $\text{err}_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$
   3) Compute $\alpha_m = \frac{1}{2} \log_e \left(\frac{1-\text{err}_m}{\text{err}_m} \right)$
   4) For samples which were predicted correctly: $w_i = w_i e^{-\alpha_m}$
   5) For samples which were predicted incorrectly: $w_i = w_i e^{\alpha_m}$
   6) Normalize w_i's to sum to 1.

Boosting : AdaBoost



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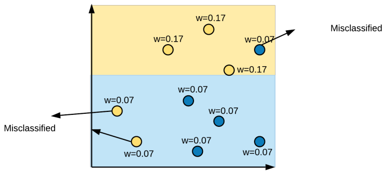

$$err_2 = \frac{0.21}{1}$$
$$\alpha_2 = \frac{1}{2} log \left(\frac{1 - 0.21}{0.21} \right) = 0.66$$

Boosting : AdaBoost

Consider we have a dataset of N samples.
Sample i has weight w_i. There are M classifiers in the ensemble.

1. Initialize weights of data samples: $w_i = \frac{1}{N}$
2. For $m = 1, \ldots, M$:
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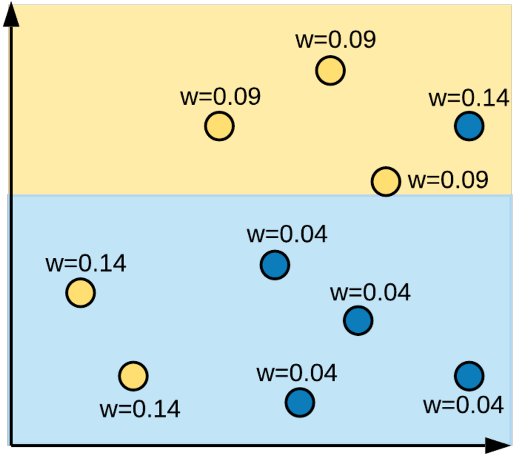
Boosting : AdaBoost



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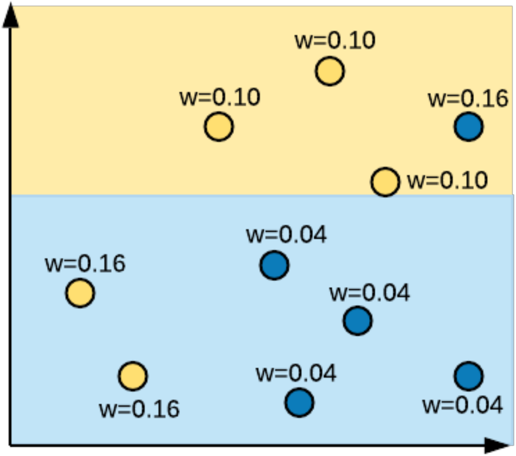
Boosting : AdaBoost



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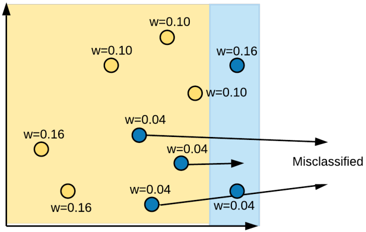


$$err_3 = \frac{0.12}{1}$$

$$\alpha_3 = \frac{1}{2} log \left(\frac{1 - 0.12}{0.12} \right) = 0.99$$

Boosting: Adaboost

Intuitively, after each iteration, importance of wrongly classified samples is increased by increasing their weights and importance of correctly classified samples is decreased by decreasing their weights.

Boosting: Adaboost

Testing

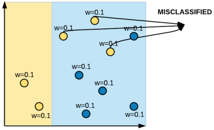
- For each sample x, compute the prediction of each classifier $h_m(x)$.
- Final prediction is the sign of the sum of weighted predictions, given as:
- $\mathrm{SIGN}(\alpha_1 h_1(x) + \alpha_2 h_2(x) + \ldots + \alpha_M h_M(x))$

Boosting: Adaboost

Example

Boosting: Adaboost

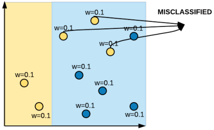
Example



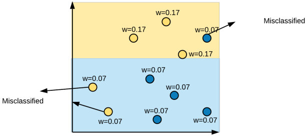
$\alpha_1 = 0.42$

Boosting: Adaboost

Example



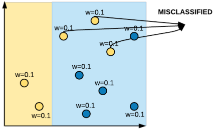
$\alpha_1 = 0.42$



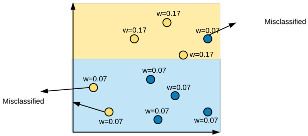
$\alpha_2 = 0.66$

Boosting: Adaboost

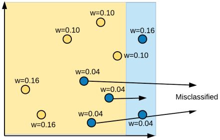
Example



$\alpha_1 = 0.42$



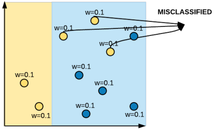
$\alpha_2 = 0.66$



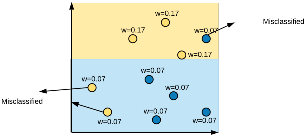
$\alpha_3 = 0.99$

Boosting: Adaboost

Example



$\alpha_1 = 0.42$



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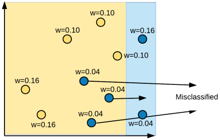
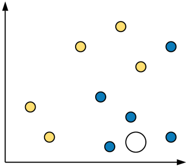
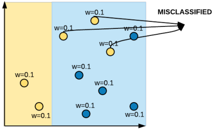


$\alpha_3 = 0.99$



Boosting: Adaboost

Example



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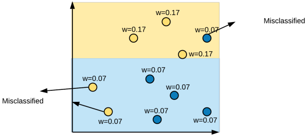

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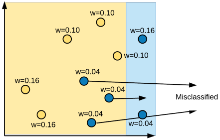

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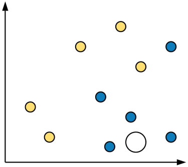
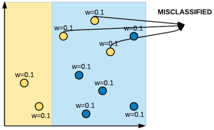


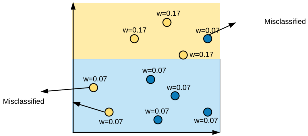
Let us say, yellow class is $+1$ and blue class is -1

Boosting: Adaboost

Example



$\alpha_1 = 0.42$



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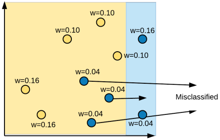

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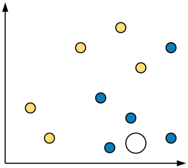


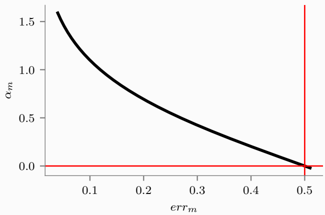
Let us say, yellow class is +1 and blue class is -1

Prediction = SIGN(0.42*-1 + 0.66*-1 + 0.99*+1) = Negative = blue

Intuition behind weight update formula

Intuition behind weight update formula

Notebook: boosting-explanation.html



Intuition behind weight update formula

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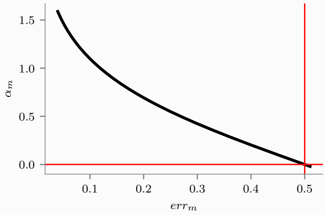
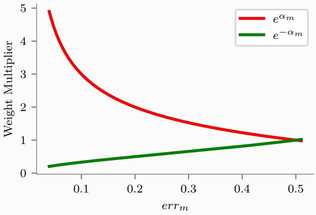


Notebook: boosting-explanation.html



ADABoost for regresion

From Paper: Improving Regressors using Boosting Techniques

Our problem will be that the modeling error is also nonzero because we have to determine the model in the presence of noise. Since we don't know the probability distributions, we approximate the expectation of the ME and PE using the sample ME (if the truth is known) and sample PE and then average over multiple experiments.

In the following discussion, we detail both bagging and boosting. We then discuss how to build trees which are the basic building blocks of our regression machines and use these ensembles on some standard test functions.

2. BAGGING

The following is a paraphrase of Breiman (1996b) with some difference in notation. Suppose we pick with replacement N_1 examples from the training set of size N_1 and call the k'th set of observations O_k. Based on these observations, we form a predictor $y^{(p)}(\boldsymbol{x},O_k)$. Because we are sampling with replacement, we may have multiple observations or no observations of a particular training example. Sampling with replacement is sometimes termed bootstrap sampling [Efron and Tibshirani (1993)] and therefore this method is called **b**ootstrap **agg**regating or bagging for short. The ensemble predictor is formed from the approximation to the expectation over all the observation sets, i.e. $E_O[y^{(p)}(\boldsymbol{x},O)]$ by using the average of the outputs of all the predictors. Breiman discusses which algorithms are good candidates for predictors and concludes that the best predictors are unstable, i.e., a small change in the training set O_k causes a large change in the predictor $y^{(p)}(\boldsymbol{x},O_k)$. Good candidates are regression trees and neural nets.

3. BOOSTING

In bagging, each training example is equally likely to be picked. In boosting, the probability of a particular example being in the training set of a particular machine depends on the performance of the prior machines on that example. The following is a modification of *Adaboost.R* [Freund and Schapire (1996a)].

Initially, to each training pattern we assign a weight $w_i=1 \quad i=1,\ldots,N_1$

Repeat the following while the average loss $\bar{L}$ defined

set. Each machine makes a hypothesis: $h_t\!:\!x\rightarrow y$

3. Pass *every* member of the training set through this machine to obtain a prediction $y_i^{(p)}(\boldsymbol{x}_i) \quad i=1,\ldots N_1$.

4. Calculate a loss for each training sample $L_i = L\left[\,|\,y_i^{(p)}(\boldsymbol{x}_i)-y_i\,|\,\right]$. The loss L may be of any functional form as long as $L\in[0,1]$. If we let

$$D = sup\,|\,y_i^{(p)}(\boldsymbol{x}_i) - y_i\,| \quad i=1,\ldots,N_1$$

then we have three candidate loss functions:

$$L_i = \frac{|\,y_i^{(p)}(\boldsymbol{x}_i) - y_i\,|}{D} \qquad (linear)$$

$$L_i = \frac{|\,y_i^{(p)}(\boldsymbol{x}_i) - y_i\,|^2}{D^2} \qquad (square\ \ law)$$

$$L_i = 1 - exp\left[\frac{-\,|\,y_i^{(p)}(\boldsymbol{x}_i) - y_i\,|}{D}\right] \qquad (exponential)$$

5. Calculate an average loss: $\bar{L} = \sum_{i=1}^{N_1} L_i p_i$

6. Form $\beta = \frac{\bar{L}}{1-\bar{L}}$. β is a measure of confidence in the predictor. Low β means high confidence in the prediction.

7. Update the weights: $w_i \rightarrow w_i\beta^{**}[1-L_i]$, where ** indicates exponentiation. The smaller the loss, the more the weight is reduced making the probability smaller that this pattern will be picked as a member of the training set for the next machine in the ensemble.

8. For a particular input $\boldsymbol{x}_i$, each of the T machines makes a prediction h_t, $t=1,\ldots,T$. Obtain the cumulative prediction h_f using the T predictors:

Random Forest

- Random Forest is an ensemble of decision trees.
- We have two types of bagging: bootstrap (on data) and random subspace (of features).
- As features are randomly selected, we learn decorrelated trees and helps in reducing variance.

Random Forest

There are 3 parameters while training a random forest number of trees, number of features (m), maximum depth.

Training Algorithm

- For i^{th} tree ($i \in \{1 \cdots N\}$), select n samples from total N samples with replacement.
- Learn Decision Tree on selected samples for i^{th} round.

Learning Decision Tree (for RF)

- For each split, select m features from total available M features and train a decision tree on selected features

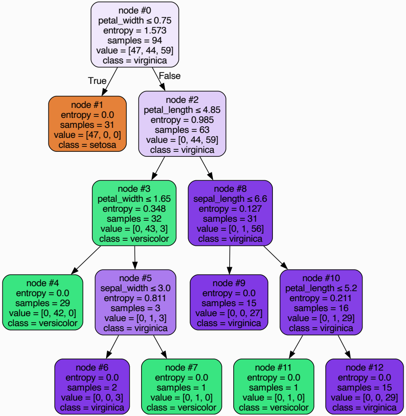
Dataset

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

150 rows × 5 columns

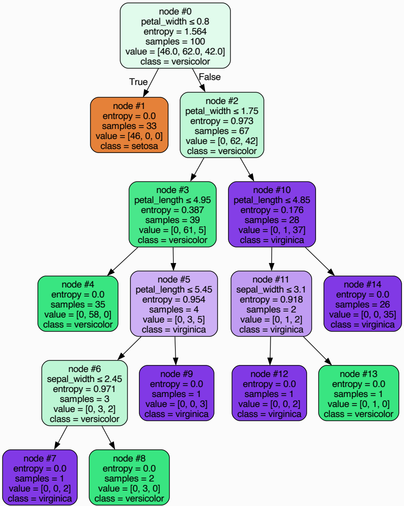
Decision Tree # 0

Notebook: ensemble-feature-importance.html



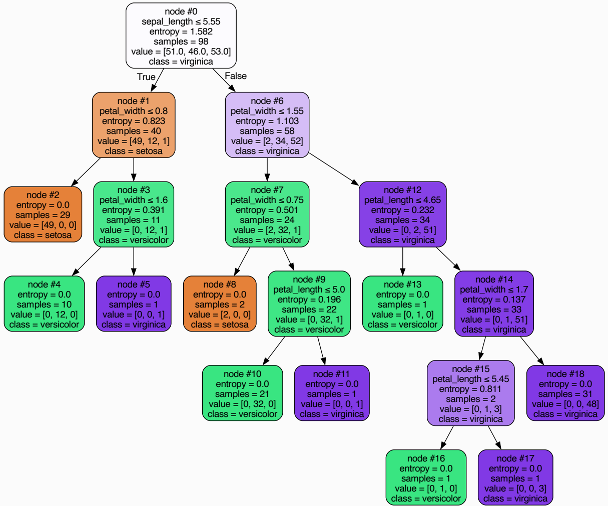
Decision Tree # 1

Notebook: ensemble-feature-importance.html



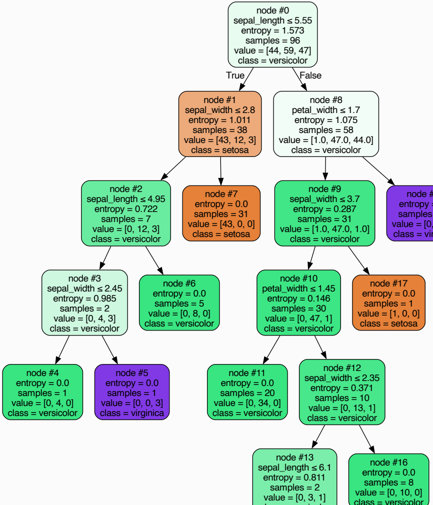
Decision Tree # 2

Notebook: ensemble-feature-importance.html



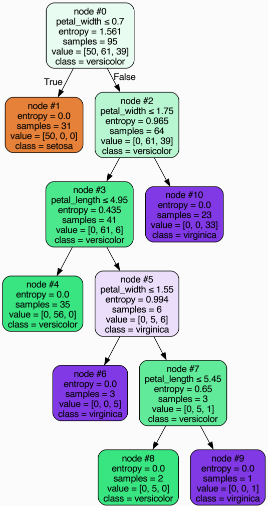
Decision Tree # 3

Notebook: ensemble-feature-importance.html



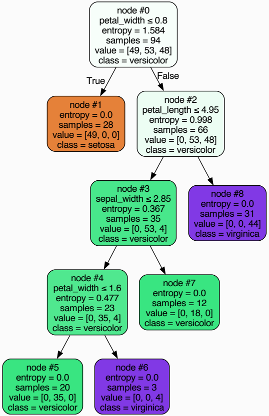
Decision Tree # 4

Notebook: ensemble-feature-importance.html



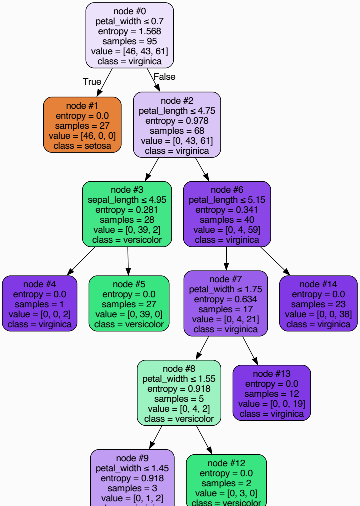
Decision Tree # 5

Notebook: ensemble-feature-importance.html



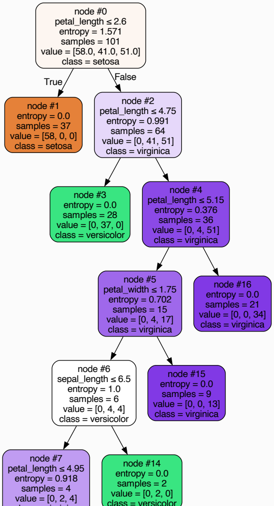
Decision Tree # 6

Notebook: ensemble-feature-importance.html



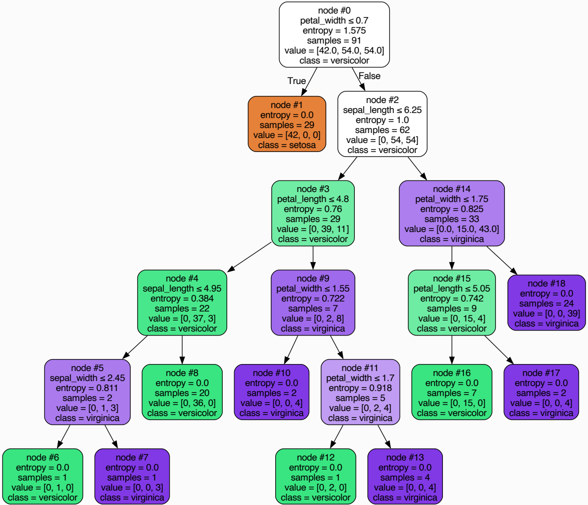
Decision Tree # 7

Notebook: ensemble-feature-importance.html



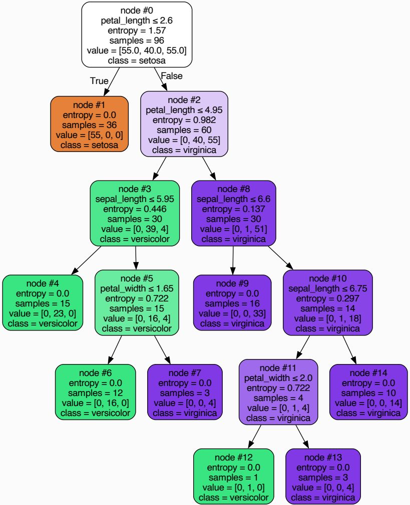
Decision Tree # 8

Notebook: ensemble-feature-importance.html

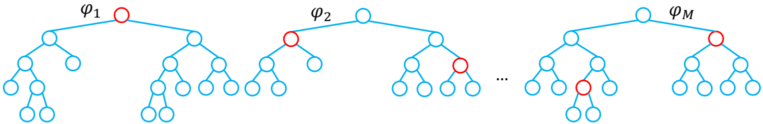


Decision Tree # 9

Notebook: ensemble-feature-importance.html



Feature Importance[1]



Importance of variable X_j for an ensemble of M trees φ_m is:

$$\text{Imp}(X_j) = \frac{1}{M} \sum_{m=1}^{M} \sum_{t \in \varphi_m} 1(j_t = j) \Big[p(t) \Delta i(t) \Big],$$

where j_t denotes the variable used at node t, $p(t) = N_t / N$ and $\Delta i(t)$ is the impurity reduction at node t:

$$\Delta i(t) = i(t) - \frac{N_{t_L}}{N_t} i(t_L) - \frac{N_{t_r}}{N_t} i(t_R)$$

[1] Slide Courtesy Gilles Louppe

Computed Feature Importance

Notebook: ensemble-feature-importance.html